

Hole spin relaxation in semiconductor quantum dots

C. Lü,^{1,2} J. L. Cheng,² and M. W. Wu^{1,2,*}

¹*Hefei National Laboratory for Physical Sciences at Microscale,
University of Science and Technology of China, Hefei, Anhui, 230026, China*

²*Department of Physics, University of Science & Technology of China, Hefei, Anhui, 230026, China[†]*
(Dated: February 2, 2008)

Hole spin relaxation time due to the hole-acoustic phonon scattering in GaAs quantum dots confined in quantum wells along (001) and (111) directions is studied after the exact diagonalization of Luttinger Hamiltonian. Different effects such as strain, magnetic field, quantum dot diameter, quantum well width and the temperature on the spin relaxation time are investigated thoroughly. Many features which are quite different from the electron spin relaxation in quantum dots and quantum wells are presented with the underlying physics elaborated.

PACS numbers: 68.65.Hb, 63.22.+m, 63.20.Ls, 71.15.-m

I. INTRODUCTION

Recently, considerable interests have been devoted to spin-related phenomena in semiconductors due to the enormous potential of the spintronic devices.^{1,2} Among these, properties of electron spins confined in semiconductor quantum dots (QD's) are essential to the proposed qubits in quantum computers and have therefore caused much attention.^{3,4,5,6,7,8} Many works calculated the spin relaxation time (SRT) of electrons due to the spin-orbit coupling induced spin-flip electron-phonon scattering at very low temperatures,^{5,7,8,9} where the dominant electron-phonon scattering arises from the piezoelectric potential. These works are based on perturbation theory where the spin-orbit coupling is treated as a perturbation in the Hilbert space spanned by H_0 which does not include the spin-orbit coupling. Moreover only the lowest few energy levels of H_0 are included in the theory. Recently we have shown that the perturbation method is inadequate in accounting for the electron structure and therefore the SRT in semiconductor QD's: The SRT obtained from the perturbation approach used in the literature^{5,7,8,9} is several orders of magnitude smaller than the exact value.¹⁰ Very recently Wood *et al.* investigated the SRT of a hole in QD's.¹¹ Again perturbation method is used and only the SRT induced by the electron-phonon scattering due to the deformation potential is considered. Many other effects such as strain, quantum well orientation and multi-subband effects as well as the effect from the electron-phonon scattering due to the piezoelectric coupling, have not been studied in their work.

In the present paper, we investigate the hole SRT of GaAs QD's confined in quantum wells along (001) and (111) directions by parabolic potentials with strain included by exactly diagonalizing the hole Hamiltonian. We calculate the hole SRT due to the scattering with acoustic phonons by the Fermi golden rule after getting the hole energy spectra and the wavefunctions from the exact diagonalization. We discuss how the strain, QD radius, magnetic field, temperature and quantum well

width affect the SRT. We show that strain on quantum wells of different growth directions affects the QD spin relaxation in totally different ways: for QD's in (001) quantum well strain changes the relative position of energy levels of heavy hole and light hole; but for those in (111) quantum well, strain makes additional spin mixing and induces additional spin relaxation. Also we show that unlike the case of electrons where the SRT is mainly determined by the electron-phonon scattering due to the piezoelectric interactions, for holes both the hole-phonon coupling due to piezoelectric interaction and that due to deformation potential make important contributions to the spin relaxation process, although their relative importance changes under different conditions.

The paper is organized as follows: In Sec. II we set up our model and Hamiltonian. In Sec. III we present our numerical results. We discuss the SRT of QD's in (001) quantum well in Sec. III(A). We first discuss a simple case: a small QD without strain where we compare our results with those obtained from the perturbation method. Then we discuss strain dependence of the SRT when the confinement of the quantum well is very strong and there is only one subband. We finish Sec. III(A) by showing the strain, magnetic field, and QD radius dependence of the SRT in the case of large well width (multi-subband effects). Then we turn to the case of QD's in (111) quantum well in Sec. III(B). In Sec. III(C) we show the well width dependence of the SRT in both (001) and (111) quantum wells. We conclude in Sec. IV.

II. MODEL AND HAMILTONIAN

We use a simplified model to study the spin relaxation in QD's which are confined by parabolic potentials $V_c(\mathbf{r})$ in a quantum well of width a . Due to the confinement of the quantum well, the momentum states along z axis are quantized. With the hard-wall approximation, the hole momentum states along z -axis are therefore characterized by the subband index n_z . The total Hamiltonian is given

by

$$H = H_h + H_{strain} + H_{ph} + H_{int} , \quad (1)$$

in which H_h is the 4×4 Luttinger Hamiltonian for holes. When the growth direction of the quantum well is along

$$H_h = \frac{1}{2m_0} \begin{pmatrix} P+Q+3\hbar e B \kappa & S & R & 0 \\ S^\dagger & P-Q-\hbar e B \kappa & 0 & R \\ R^\dagger & 0 & P-Q+\hbar e B \kappa & -S \\ 0 & R^\dagger & -S^\dagger & P+Q-3\hbar e B \kappa \end{pmatrix} + V_c(\mathbf{r}) , \quad (2)$$

in which

$$V_c(\mathbf{r}) = \begin{pmatrix} \frac{1}{2} m_{h\parallel}^{001} (\omega_h^{001})^2 r^2 & 0 & 0 & 0 \\ 0 & \frac{1}{2} m_{l\parallel}^{001} (\omega_l^{001})^2 r^2 & 0 & 0 \\ 0 & 0 & \frac{1}{2} m_{l\parallel}^{001} (\omega_l^{001})^2 r^2 & 0 \\ 0 & 0 & 0 & \frac{1}{2} m_{h\parallel}^{001} (\omega_h^{001})^2 r^2 \end{pmatrix} , \quad (3)$$

and

$$P \pm Q = (\gamma_1 \pm \gamma_2)[P_x^2 + P_y^2] + (\gamma_1 \mp 2\gamma_2) \frac{\hbar^2 \pi^2 n_z^2}{a^2} \delta_{n_z, n'_z} , \quad (4)$$

$$S = -2\sqrt{3}\gamma_3 \frac{4i\hbar n'_z n_z}{a[(n'_z)^2 - (n_z)^2]} (1 - \delta_{n_z, n'_z}) \times [P_x - iP_y] , \quad (5)$$

$$R = -\sqrt{3}\{\gamma_2[P_x^2 - P_y^2] - 2i\gamma_3 P_x P_y\} . \quad (6)$$

In these equations, m_0 denotes free electron mass; γ_1 , γ_2 , γ_3 and κ are Luttinger coefficients; and n_z and n'_z represent the subband indices. ω_h^{001} and ω_l^{001} in the two dimensional confinement potential $V_c(\mathbf{r})$ [Eq. (3)] represent the confinements experienced by the heavy hole and light hole respectively and are given by $\omega_h^{001} = \hbar/(m_{h\parallel}^{001} d^2)$ and $\omega_l^{001} = \hbar/(m_{l\parallel}^{001} d^2)$, with $m_{h\parallel}^{001} = m_0/(\gamma_1 + \gamma_2)$ and $m_{l\parallel}^{001} = m_0/(\gamma_1 - \gamma_2)$ standing for the effective masses of heavy hole and light hole in the direction perpendicular to the growth (001) direction and d representing the QD diameter. By applying a magnetic field \mathbf{B} along the growth (z) direction of the quantum well and adopting the Coulomb gauge $\mathbf{A} = (-\frac{By}{2}, \frac{Bx}{2}, 0)$, one has $P_x = (\hbar k_x + \frac{eBy}{2})$ and $P_y = (\hbar k_y - \frac{eBx}{2})$.

From the Luttinger Hamiltonian Eq. (2) one can see that when the well width a is sufficiently small and only the lowest subband in QD is important, $S = 0$ and $+\frac{3}{2}$ ($-\frac{3}{2}$) states can only mix with $-\frac{1}{2}$ ($+\frac{1}{2}$) states. Therefore there is no mixing between the spin-up and -down ($\pm\frac{3}{2}$) heavy hole states and between the spin-up and -down ($\pm\frac{1}{2}$) light hole states. Spin mixing between the spin-up heavy hole and the spin-down light hole or *vice versa* is negligible as the energy difference between the heavy hole

the (001) direction (z -axis) and the matrix elements are arranged in the order of $J_z = +\frac{3}{2}$, $+\frac{1}{2}$, $-\frac{1}{2}$ and $-\frac{3}{2}$, H_h can be written as¹³

and light hole states is usually too large. Nevertheless for larger well width where higher subbands are needed, S no longer equals to zero and the spin-up and -down heavy-hole states are mixed with each other, mediated by the light-hole states. The same is true for the spin-up and -down light-hole states.

The strain Hamiltonian H_{strain} given by the Bir-Pikus Hamiltonian¹⁴ has the form:

$$H_{strain} = \begin{pmatrix} F & H & I & 0 \\ H^\dagger & G & 0 & I \\ I^\dagger & 0 & G & -H \\ 0 & I^\dagger & -H^\dagger & F \end{pmatrix} \quad (7)$$

with the matrix elements being

$$F = -(D_a + \frac{D_b}{2})\text{Tr}(\epsilon) + \frac{3D_b}{2}\epsilon_{zz} , \quad (8)$$

$$G = -(D_a - \frac{D_b}{2})\text{Tr}(\epsilon) - \frac{3D_b}{2}\epsilon_{zz} , \quad (9)$$

$$H = D_d(\epsilon_{zx} - i\epsilon_{zy}) , \quad (10)$$

$$I = \frac{\sqrt{3}}{2}D_b(\epsilon_{xx} - \epsilon_{yy}) - iD_d\epsilon_{xy} . \quad (11)$$

Here D_a , D_b and D_d are the deformation potential constants. ϵ is the strain tensor with ϵ_{ij} denoting the tensor components. For (001)-oriented zinc blende crystal the strain tensor components are given by¹⁵

$$\epsilon_{xx}^{001} = \epsilon_{yy}^{001} = \epsilon_{\parallel} = \frac{a_2 - a_1}{a_1} \quad (12)$$

$$\epsilon_{zz}^{001} = -2\frac{C_{12}}{C_{11}}\epsilon_{\parallel} \quad (13)$$

$$\epsilon_{xy}^{001} = \epsilon_{yz}^{001} = \epsilon_{zx}^{001} = 0 , \quad (14)$$

where a_1 and a_2 are the lattice constants of epilayer (GaAs) and substrate materials, and C_{11} and C_{12} are the stiffness constants. One can see that for (001)-oriented zinc blende crystal, $H = I = 0$ and the strain Hamiltonian Eq. (7) has only the diagonal terms. Therefore the strain does not induce any extra spin mixing, but adjusts

the relative positions of the heavy-hole and light-hole energy levels.

When the growth direction of the quantum well (z -axis) is along (111) direction, the hole Luttinger Hamiltonian H_h is the same as that in Eq. (2), but with the matrix elements being replaced by¹³

$$P \pm Q = (\gamma_1 \pm \gamma_3)[P_x^2 + P_y^2] + (\gamma_1 \mp 2\gamma_3)\frac{\hbar^2\pi^2 n_z^2}{a^2}\delta_{n_z, n'_z}, \quad (15)$$

$$S = \frac{\sqrt{6}}{3}(\gamma_2 - \gamma_3)[P_x + iP_y]^2 - \frac{2\sqrt{3}}{3}(2\gamma_2 + \gamma_3)\frac{4i\hbar n'_z n_z}{a[(n'_z)^2 - (n_z)^2]}(1 - \delta_{n_z, n'_z})[P_x - iP_y], \quad (16)$$

$$R = -\frac{\sqrt{3}}{3}(\gamma_2 + 2\gamma_3)[P_x - iP_y]^2 + \frac{2\sqrt{6}}{3}[(\gamma_2 - \gamma_3)\frac{4i\hbar n'_z n_z}{a[(n'_z)^2 - (n_z)^2]}(1 - \delta_{n_z, n'_z})[P_x + iP_y]]. \quad (17)$$

Moreover ω_h^{001} , ω_l^{001} , $m_{||}^{001}$ and $m_{h||}^{001}$ in Eq. (3) should be replaced by ω_h^{111} , ω_l^{111} , $m_{||}^{111}$ and $m_{h||}^{111}$, which are given by $\omega_h^{111} = \hbar/(m_{h||}^{111}d^2)$ and $\omega_l^{111} = \hbar/(m_{||}^{111}d^2)$, $m_{h||}^{111} = m_0/(\gamma_1 + \gamma_3)$ and $m_{||}^{111} = m_0/(\gamma_1 - \gamma_3)$ respectively. From Eqs. (15-17), one finds that differing from the previous (001) case, here S and R are nonzero even for the single subband case. This means when the growth direction is along (111) crystal direction, there is always mixing between the spin-up and -down heavy-hole states and the spin-up and -down light-hole states.

The strain Hamiltonian H_{strain} for (111)-oriented zinc blende crystal is same as that in Eqs. (7-11), but now the strain tensor components are given by¹⁵

$$\epsilon_{xx}^{111} = \epsilon_{yy}^{111} = \epsilon_{zz}^{111} = \frac{1}{3}(2 - 1/\sigma^{111})\epsilon_{||}, \quad (18)$$

$$\epsilon_{xy}^{111} = \epsilon_{yz}^{111} = \epsilon_{zx}^{111} = -\frac{1}{3}(1 + 1/\sigma^{111})\epsilon_{||}, \quad (19)$$

$$\sigma^{111} = \frac{C_{11} + 3C_{12} + 4C_{44}}{2C_{11} + 4C_{12} - 4C_{44}}, \quad (20)$$

with C_{44} the stiffness constant. Substituting Eqs. (18-20) into Eqs. (7-11), one gets $F = G$ and the off-diagonal elements H and I are no longer equal to zero. Consequently when one applies a strain on (111)-oriented zinc blende quantum well, the change of energy levels of the light and heavy holes are almost the same and the strain introduces additional spin mixing between the spin-up and -down heavy/light holes.

H_{ph} in Eq. (1) is the Hamiltonian of acoustic phonons and is given by $H_{ph} = \sum_{\mathbf{Q}\lambda} \hbar\omega_{\mathbf{Q}\lambda} a_{\mathbf{Q}\lambda}^\dagger a_{\mathbf{Q}\lambda}$ with $\omega_{\mathbf{Q}\lambda}$ standing for the phonon energy spectrum of branch λ and momentum \mathbf{Q} . Two different hole-phonon scattering mechanisms contribute to the spin relaxation for the temperatures we consider here. One is hole-phonon scattering due to piezoelectric coupling which is given by

$$H_{int}^{pie} = \sum_{\mathbf{Q}\lambda} M_{\mathbf{Q}\lambda} (a_{-\mathbf{Q}\lambda}^\dagger + a_{\mathbf{Q}\lambda}) \exp(i\mathbf{Q} \cdot \mathbf{r}) \quad (21)$$

with $M_{\mathbf{Q}\lambda}$ being the scattering the matrix elements. For longitudinal acoustic phonons $M_{\mathbf{Q}pl}^2 = \frac{32\pi^2 e^2 e_{14}^2}{\epsilon^2 \rho v_{sl}} \frac{(3Q_x Q_y Q_z)^2}{Q^2}$ and for two transverse acoustic phonons $\sum_{j=1,2} M_{\mathbf{Q}ptj}^2 = \frac{32\pi^2 e^2 e_{14}^2}{\epsilon^2 \rho v_{st} Q^5} [Q_x^2 Q_y^2 + Q_y^2 Q_z^2 + Q_z^2 Q_x^2 - \frac{(3Q_x Q_y Q_z)^2}{Q^2}]$. Here ρ is the GaAs volume density, e_{14} represents the piezoelectric coupling constant and ϵ denotes the static dielectric constant. The acoustic phonon energy spectra $\omega_{\mathbf{Q}\lambda}$ are given by $\omega_{\mathbf{Q}l} = v_{sl}Q$ for the longitudinal mode and $\omega_{\mathbf{Q}pt} = v_{st}Q$ for the transverse mode with v_{sl} and v_{st} standing for the corresponding sound velocities. $Q = \sqrt{Q_x^2 + Q_y^2 + Q_z^2}$. It is noted that this kind of scattering *does not* flip hole spin and therefore only when the hole wave function itself contains spin mixing can H_{int}^{pie} contributes to spin relaxation. The other is hole-phonon scattering due to the deformation potential H_{int}^{def} . H_{int}^{def} can be derived from H_{strain} Eq. (7) by substituting ϵ_{ij} in Eqs. (8-11) by $\epsilon_{ij} = \epsilon_{ij}^0 + \epsilon'_{ij}$, and splitting H_{strain} into two parts: one contains all terms proportional to ϵ_{ij}^0 and the other contains all terms proportional to ϵ'_{ij} .¹¹ The second part is therefore H_{int}^{def} if ϵ_{ij}^0 represent the strain tensor components caused by the sample and ϵ'_{ij} are the tensor components caused by the lattice vibrations. ϵ'_{ij} can further be written in terms of normal-mode coordinates as

$$\epsilon'_{ij} = \sum_{\mathbf{Q}\lambda} \frac{i}{2} \sqrt{\frac{\hbar}{2\rho V \omega_{\mathbf{Q}\lambda}}} (a_{\mathbf{Q}\lambda} + a_{-\mathbf{Q}\lambda}^\dagger) \times (\hat{\eta}_{i\lambda} Q_j + \hat{\eta}_{j\lambda} Q_i) e^{i\mathbf{Q} \cdot \mathbf{r}}, \quad (22)$$

with ρ being the mass density of the material, \mathbf{Q} standing for the phonon wave vector and $\hat{\eta}_{i\lambda}$ representing the unit vector of polarization of λ -phonon along i -direction. For longitudinal mode $\hat{\eta}_i = Q_i/Q$ and for two transverse modes $\hat{\eta}_{11} = (Q_x Q_z, Q_y Q_z, -Q_\perp^2)/Q Q_\perp$ and $\hat{\eta}_{12} = (Q_y, -Q_x, 0)/Q_\perp$ with $Q_\perp = \sqrt{Q_x^2 + Q_y^2}$.¹¹ It is

pointed out that H_{int}^{def} is spin-flip scattering as it contains non-zero off-diagonal parts H and I , and therefore can cause spin relaxation even for the case when there is no spin mixing in the wavefunctions. Accounting for these two hole-phonon scattering mechanisms, one has $H_{int} = H_{int}^{pie} + H_{int}^{def}$.

We diagonalize the Luttinger Hamiltonian H_h in the Hilbert space $|n, l, n_z, \sigma\rangle$ constructed by H_0 which is taken to be the diagonal part of H_h :

$$|\Psi_\ell\rangle = \sum_{nl n_z \sigma} C_{nl n_z \sigma}^\ell |n, l, n_z, \sigma\rangle. \quad (23)$$

Here $H_0|n, l, n_z, \sigma\rangle = E_{n, l, n_z, \sigma}^\xi |n, l, n_z, \sigma\rangle$ with

$$\begin{aligned} \langle \mathbf{r} | n, l, n_z, \sigma \rangle &= N_{n, l} (\sqrt{\alpha} r)^{|l|} e^{-\frac{\alpha r^2}{2}} L_n^{|l|}(\alpha r^2) e^{i l \theta} \\ &\times \sqrt{\frac{2}{a}} \sin\left(\frac{n_z \pi}{a} z\right), \end{aligned} \quad (24)$$

$$\begin{aligned} E_{n, l, n_z, \pm \frac{3}{2}}^\xi &= \frac{m_0}{m_{h\parallel}^\xi} [\hbar \Omega (2n + |l| + 1) - \hbar \omega_B l] \\ &\pm \frac{3 \hbar e B \kappa}{2 m_0} + \frac{m_0}{m_{hz}^\xi} \frac{\hbar^2 \pi^2 n_z^2}{2 m_0 a^2}, \end{aligned} \quad (25)$$

$$\begin{aligned} E_{n, l, n_z, \pm \frac{1}{2}}^\xi &= \frac{m_0}{m_{l\parallel}^\xi} [\hbar \Omega (2n + |l| + 1) - \hbar \omega_B l] \\ &\pm \frac{\hbar e B \kappa}{2 m_0} + \frac{m_0}{m_{lz}^\xi} \frac{\hbar^2 \pi^2 n_z^2}{2 m_0 a^2}. \end{aligned} \quad (26)$$

In these equations $n = 0, 1, 2, \dots$ and $l = 0, \pm 1, \pm 2, \dots$ are quantum numbers; ξ denotes the growth direction which can be (001) or (111); m_{hz}^ξ and m_{lz}^ξ stand for the effective masses of heavy and light holes in the z -direction which are given by $m_0/m_{hz}^{001} = \gamma_1 - 2\gamma_2$, $m_0/m_{hz}^{111} = \gamma_1 - 2\gamma_3$, $m_0/m_{lz}^{001} = \gamma_1 + 2\gamma_2$ and $m_0/m_{lz}^{111} = \gamma_1 + 2\gamma_3$; $\Omega = \sqrt{\omega_0^2 + \omega_B^2}$ with $\omega_0 = \hbar/(m_0 d^2)$ and $\omega_B = eB/(2m_0)$; $N_{n, l} = \left(\frac{\alpha n!}{\pi(n+|l|)!}\right)^{\frac{1}{2}}$ with $\alpha = m_0 \Omega / \hbar$. $L_n^{|l|}$ is the generalized Laguerre polynomial.

The eigenfunction $|\Psi_\ell\rangle$ in Eq. (23) is a mixture of four different components: spin-up and -down heavy-hole and light-hole states. We assign an eigenstate ℓ to be spin up if the spin-up components are larger than the spin-down ones. An hole at initial state i with energy ϵ_i and a spin polarization can be scattered by the phonon into another state f with energy ϵ_f and the opposite spin polarization. The rate of such scattering can be described by the Fermi golden rule:

$$\begin{aligned} \Gamma_{i \rightarrow f} &= \frac{2\pi}{\hbar} \sum_{\mathbf{Q}\lambda} |\mathcal{M}_{\mathbf{Q}\lambda}|^2 [\bar{n}_{\mathbf{Q}\lambda} \delta(\epsilon_f - \epsilon_i - \omega_{\mathbf{Q}\lambda}) \\ &+ (\bar{n}_{\mathbf{Q}\lambda} + 1) \delta(\epsilon_f - \epsilon_i + \omega_{\mathbf{Q}\lambda})], \end{aligned} \quad (27)$$

with $\bar{n}_{\mathbf{Q}\lambda}$ representing the Bose distribution of phonon with mode λ and momentum \mathbf{Q} at temperature T and $\mathcal{M}_{\mathbf{Q}\lambda}$ being the corresponding matrix elements. For hole-phonon scattering due to the piezoelectric coupling,

$|\mathcal{M}_{\mathbf{Q}\lambda}|^2 = |M_{\mathbf{Q}\lambda} \langle f | e^{i\mathbf{Q}\cdot\mathbf{r}} | i \rangle|^2$. It is noted that only when the eigenstates $|i\rangle$ and $|f\rangle$ contain spin mixing can $\mathcal{M}_{\mathbf{Q}\lambda} \neq 0$ be possible. For hole-phonon scattering due to the deformation potential, $|\mathcal{M}_{\mathbf{Q}\lambda}|^2 = |\langle f | H_{\mathbf{Q}\lambda} | i \rangle|^2$ with $H_{\mathbf{Q}\lambda}$ the matrix for the hole-deformation potential. As $H_{\mathbf{Q}\lambda}$ itself contains spin mixing, therefore it is not necessary to have spin-mixed initial and final states to ensure $\mathcal{M}_{\mathbf{Q}\lambda} \neq 0$. The total SRT τ can be written as

$$\frac{1}{\tau} = \sum_i f_i \sum_f \Gamma_{i \rightarrow f}, \quad (28)$$

in which $f_i = C \exp[-\epsilon_i/(k_B T)]$ denotes the Maxwell distribution of the i -th level with C being a constant.

III. NUMERICAL RESULTS

It is seen from our previous discussion that hole spin relaxation in QD's is very complicated and is affected by many effects. When the quantum well is along (001) direction, for small well width (with only the lowest subband) only hole-phonon scattering due to deformation potential contributes to the spin relaxation; for large well width (with multi subbands) hole-phonon scattering due to both deformation potential and piezoelectric coupling contributes to the spin relaxation. Strain itself in this case cannot bring additional spin relaxation but influences it by changing or even reversing the relative positions of energy levels of heavy hole and light hole. Especially when a minus strain makes the energy levels of heavy hole and light hole very close to each other, spin mixing between spin-up (-down) heavy hole and spin-down (-up) light hole cannot be neglected anymore and therefore the hole-phonon scattering due to piezoelectric coupling may contribute to spin relaxation also. Nevertheless, when the quantum well is along (111) direction, regardless of the well width, there exists spin mixing between spin-up and -down heavy (light) holes in the eigenfunctions of the Luttinger Hamiltonian. Therefore hole-phonon scattering due to both deformation potential and piezoelectric coupling contributes to the spin relaxation. Moreover, strain itself in this case makes additional spin mixing and induces additional spin relaxation. In this section we perform a comprehensive investigation to find out the relative importance of above mentioned effects under various conditions such as temperature, magnetic field, QD radius and quantum well width. The parameters used in the computation are listed in Table I.^{14,16,17}

In order to ensure the convergence of the energy spectra ϵ_ℓ , we use sufficient basis functions to diagonalize the hole Hamiltonian H_h . For example, in a QD with $B = 1$ T, $a = 5$ nm, $d = 20$ nm and without strain one has to use 100 basis functions to converge the lowest 40 levels; Nevertheless, when $a = 20$ nm one has to use 484 basis functions to converge the same levels.

ρ	$5.3 \times 10^3 \text{ kg/m}^3$	ϵ	12.9	γ_1	6.85
v_{st}	$2.48 \times 10^3 \text{ m/s}$	D_a	-6.7 eV	γ_2	2.1
v_{sl}	$5.29 \times 10^3 \text{ m/s}$	D_b	-1.7 eV	γ_3	2.9
e_{14}	$1.41 \times 10^3 \text{ V/m}$	D_d	-4.55 eV	κ	1.2
C_{11}	11.81	C_{12}	5.32	C_{44}	5.94

TABLE I: Parameters used in the calculation.

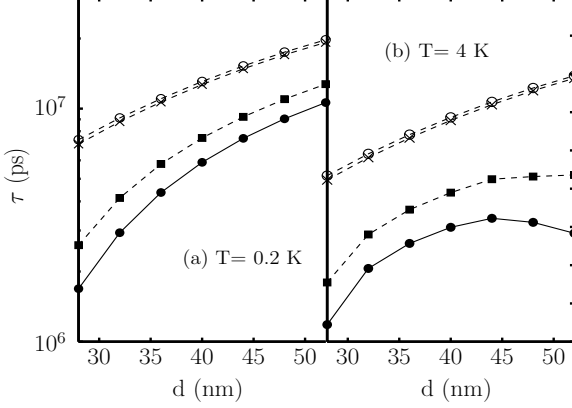


FIG. 1: SRT *vs.* QD diameter d . Curve with \bullet : exact diagonalization result with the energy sufficiently converged; Curve with \times : Perturbation result; Curve with \circ : exact diagonalization result but with only the lowest two heavy hole and the lowest two light hole levels used as basis functions. Curve with \blacksquare : exact diagonalization result but with only the 16 energy levels of H_0 given in the text as basis functions. (a): $T = 0.2$ K and (b): $T = 4$ K.

A. QD's in (001) quantum well

1. Small well width without strain

We first consider QD's in a small (001) quantum well ($a = 5$ nm) without any strain where the lowest eigen states of H_0 are heavy holes and the separation between the heavy and light holes is around 0.1 eV. Due to the small well width, only the lowest subband is needed in the calculation. Therefore, as pointed out above, only the hole-phonon scattering due to the deformation potential contributes to the spin relaxation.

In Fig. 1 we plot the SRT as a function of the QD diameter for two temperatures. $B = 1$ T in the calculation. Curves with \bullet are the results obtained by the exact diagonalization method with the energy levels sufficiently converged. Unexpectedly, differing from intuition as well as the results of an electron spin in QD's,¹⁰ it shows in Fig. 1(a) that the SRT *increases* with the QD diameter.

To understand/check this result, we compare the results from the exact diagonalization method with those from the perturbation approach widely used in the literature,^{5,7,8,9} but with the proper modification by including the second order corrections to the energy spectrum as pointed out in our previous work.¹⁰ Here we

treat the off-diagonal part of Luttinger Hamiltonian H_h as perturbation and calculate the SRT between the lowest two energy levels composed by two lowest heavy hole and two lowest light hole states of H_0 : $|0, 0, 1, \sigma\rangle$ with $\sigma = \pm\frac{3}{2}$ and $\pm\frac{1}{2}$. The wave functions can be written as:

$$\begin{aligned} \langle \mathbf{r} | \Psi_{\uparrow} \rangle &= \langle \mathbf{r} | 0, 0, 1, \frac{3}{2} \rangle - \mathcal{A} \langle \mathbf{r} | 0, 0, 1, -\frac{1}{2} \rangle, \\ \langle \mathbf{r} | \Psi_{\downarrow} \rangle &= \langle \mathbf{r} | 0, 0, 1, -\frac{3}{2} \rangle - \mathcal{B} \langle \mathbf{r} | 0, 0, 1, \frac{1}{2} \rangle, \end{aligned} \quad (29)$$

in which

$$\mathcal{A} = -\frac{\sqrt{3}\gamma_3\hbar eB}{4\gamma_2\hbar^2(\pi^2/a^2 - \alpha) - 4\hbar eB\kappa}, \quad (30)$$

$$\mathcal{B} = -\frac{\sqrt{3}\gamma_3\hbar eB}{4\gamma_2\hbar^2(\pi^2/a^2 - \alpha) + 4\hbar eB\kappa}. \quad (31)$$

With the second order correction to the energy included, the energy difference between the spin-up $|\Psi_{\uparrow}\rangle$ and spin-down $|\Psi_{\downarrow}\rangle$ states can be written as:

$$\begin{aligned} \Delta E &= \frac{6\hbar eB\kappa}{2m_0} + |\mathcal{A}|^2(E_{0,0,1,\frac{3}{2}} - E_{0,0,1,-\frac{1}{2}}) \\ &\quad - |\mathcal{B}|^2(E_{0,0,1,-\frac{3}{2}} - E_{0,0,1,\frac{1}{2}}) \\ &= \frac{6\hbar eB\kappa}{2m_0} - \frac{3\kappa\gamma_3^2(\hbar eB)^3/(4m_0)}{[\gamma_2\hbar^2(\pi^2/a^2 - \alpha)]^2 - (\hbar eB\kappa)^2} \end{aligned} \quad (32)$$

in which the first term represents Zeeman splitting. The SRT τ can therefore be written as:

$$\begin{aligned} \frac{1}{\tau} &= \sum_{\lambda} \frac{D_d^2 \Delta E^3 n_{Q\lambda}}{2\pi(\hbar v_{s\lambda})^4 v_{s\lambda} \rho} \int_0^{\frac{\pi}{2}} d\theta \mathcal{K}_{\lambda}(\theta) (\mathcal{A} - \mathcal{B})^2 \\ &\quad \times \exp\left(-\frac{q^2}{2\alpha}\right) I^2(q_z), \end{aligned} \quad (33)$$

with $Q = \Delta E/(\hbar v_s)$, $q = Q \sin \theta$, $q_z = Q \cos \theta$ and $I(q_z) = 8\pi^2 \sin(aq_z/2)/\{aq_z[4\pi^2 - (aq_z)^2]\}$. λ stands for the branch of phonon: for longitude mode $\mathcal{K}_l(\theta) = \sin^3(\theta) \cos^2(\theta)$ and for two transverse modes $\mathcal{K}_{t1}(\theta) = \frac{1}{4} \sin(\theta) \cos^2(2\theta)$ and $\mathcal{K}_{t2}(\theta) = \frac{1}{4} \sin(\theta) \cos^2(\theta)$ respectively. The SRT's calculated from Eq. (33) are plotted as the curve with \times in Fig. 1(a) which coincides with the curve with \circ obtained from the exact diagonalization method but with exactly the same four basis functions used in the perturbation method as basis. One can see that the SRT τ does *increase* with the QD diameter at $T = 0.2$ K. From Eqs. (30-33) one finds that the SRT depends on the diameter only through α , which can be approximated into $\alpha = 1/d^2$ in the case $\omega_0 \gg \omega_B$. Moreover, the mixture of wave functions and the energy difference ΔE hardly change with d for $\pi^2/a^2 \gg 1/d^2$. Therefore only the exponential term $\exp(-\frac{q^2}{2\alpha})$ in Eq. (33) decreases with d . As a result larger QD diameter corresponds to longer SRT at low temperature.

As shown in our previous work that the right perturbation approach (with the second order corrections to energy spectrum included) with the lowest few levels of H_0

as basis functions may lead to totally opposite trend from the exact diagonalization method with sufficient number of basis functions.¹⁰ In order to rule out this possibility in the present analysis, we plot in Fig. 1(a) the SRT calculated from exact diagonalization method but with sixteen eigen functions of H_0 as basis functions, *i.e.*, $|0, 0, 1, \sigma\rangle$ and $|0, 1, 1, \sigma\rangle$ with $\sigma = \pm\frac{1}{2}$ and $\pm\frac{3}{2}$. It is seen from the figure that it produces the same τ - d dependence.

In Fig. 1(b) we plot the same curves but at $T = 4$ K. It is seen that at this temperature the SRT has a maximum as a function of the diameter d . This is because at high temperatures the scattering between the higher energy levels becomes important. These high energy levels are arrayed very close to each other. The increase of diameters makes more levels into the scattering channels and thus induces a faster spin relaxation if it overcomes the opposite tendency described above. The perturbation approach only includes the lowest two heavy-hole and two light-hole energy levels and therefore can not get the maximum feature here.

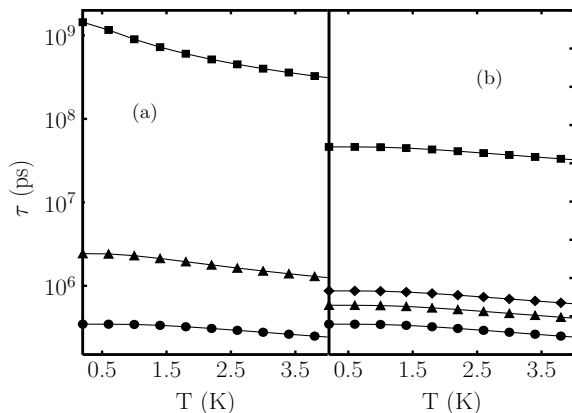


FIG. 2: SRT *vs.* temperature T for QD with $a = 5$ nm and $d = 20$ nm. (a): Results under different magnetic fields. Curve with \blacksquare : $B = 0.2$ T; Curve with \blacktriangle : $B = 0.6$ T; Curve with \bullet : $B = 1$ T. (b): Results at $B = 1$ T with contributions from different branches of phonons specified. Curve with \blacksquare : Contribution from longitudinal phonons; Curve with \blacktriangle : Contribution from the transverse phonons of first branch; Curve with \blacklozenge : Contributions from the transverse phonons of the second branch; Curve with \bullet : The total SRT.

In Fig. 2(a) we plot the SRT as a function of the temperature for a QD with $a = 5$ nm and $d = 20$ nm under three different magnetic fields. From the figure one finds that the SRT decreases with the temperature as higher temperature leads to larger number of phonons $n_{Q\lambda}$ and consequently a larger transition probability. Moreover, as pointed out in our previous work,¹⁰ smaller magnetic field makes the SRT decrease faster with the temperature. This is because the energy intervals between different energy levels are small in the presence of a small magnetic field. This leads to a faster response to the temperature. In Fig. 2(b) we further specify the contributions from different branches of phonons. It is stressed

again that only the hole-phonon scattering due to the deformation potential contributes to the spin relaxation here. As the temperature is below 4 K, the scattering from spin-up to spin-down states, in which phonons are emitted, is much larger than that from the reverse process, in which phonons are absorbed. Therefore, unless specified, the scattering rate $\frac{1}{\tau}$ is defined to be the scattering from spin-up to spin-down states throughout this paper. It is seen from the figure that the SRT here is determined by the transverse modes.

2. Small width with strain

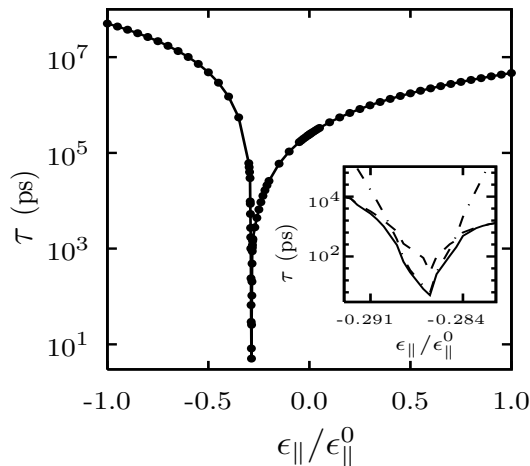


FIG. 3: SRT versus strain for a QD in (001) quantum well at $a = 5$ nm, $d = 20$ nm and $B = 1$ T at $T = 4$ K. Solid curve: total SRT; Chain curve: SRT induced by the hole-phonon scattering due to piezoelectric coupling; Dashed curve: SRT induced by the hole-phonon scattering due to deformation potential.

As pointed out in the previous section, strain on (001) quantum well can change or even reverse the relative positions of energy levels of heavy and light holes. Now we turn to investigate QD's under different strains in (001) quantum well with $a = 5$ nm, $d = 20$ nm and $B = 1$ T at $T = 4$ K. The strain is adjusted by changing the strain tensor component ϵ_{\parallel} in Eqs. (12) and (13). We plot the SRT versus $\epsilon_{\parallel}/\epsilon_{\parallel}^0$ in Fig. 3 with ϵ_{\parallel}^0 obtained by substituting the lattice constants of GaAs and InAs for a_2 and a_1 respectively in Eq. (12). It is seen from the figure that when $\epsilon_{\parallel} > 0$, the SRT τ increases with applied strain. This is because the positive strain enhances the gap between the heavy hole and light hole. Nevertheless, the flip from the spin-up heavy hole to the spin-down one is determined by the light-hole components in the wavefunctions. Increasing the gap between the heavy and light holes greatly reduces the spin relaxation and leads to the increase of SRT. When we apply a negative strain, as the gap decreases, the SRT decreases as shown in the figure. Particularly at $\epsilon_{\parallel}/\epsilon_{\parallel}^0 = -0.3$ the lowest

two energy states change from the heavy-hole states to the light-hole ones and the SRT shows a minimum. When $\epsilon_{\parallel}/\epsilon_{\parallel}^0 < -0.3$ the initial spin states are light holes and increasing strain along the negative direction enhances the gap of light hole and heavy hole again and therefore the SRT is enhanced again.

SRT around $\epsilon_{\parallel}/\epsilon_{\parallel}^0 = -0.3$ needs more address. Around this point, the energy levels of heavy hole and light hole are close to each other and therefore as said before that the hole-phonon scattering due to piezoelectric coupling is able to contribute to the spin relaxation. This can be seen in the inset of Fig. 3 where SRT due to the piezoelectric coupling is plotted as a chain curve and that due to deformation potential is plotted as dashed one. The solid curve is the total SRT. Very close to $\epsilon_{\parallel}/\epsilon_{\parallel}^0 = -0.3$, the SRT is determined by the hole-phonon scattering due to piezoelectric coupling. However, the contribution of piezoelectric coupling decays dramatically with little deviation of the strain from -0.3 . When $\epsilon_{\parallel}/\epsilon_{\parallel}^0 < -0.29$ or > -0.284 , the SRT is totally determined by the hole-phonon scattering due to the deformation potential.

3. Large width

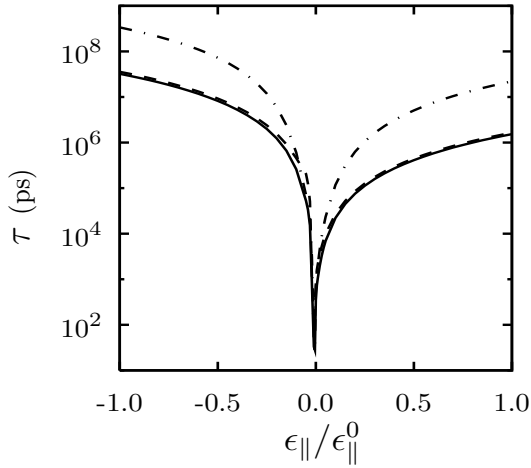


FIG. 4: SRT *vs.* strain for a QD in (001) quantum well at $a = 20$ nm, $d = 20$ nm and $B = 1$ T at $T = 4$ K. Solid curve: total SRT; Chain curve: SRT induced by the hole-phonon scattering due to piezoelectric coupling; Dashed curve: SRT induced by the hole-phonon scattering due to deformation potential.

Now we turn to investigate the SRT in a QD of $a = 20$ nm, $d = 20$ nm and $B = 1$ T at $T = 4$ K. For such a well width, one has to include states with $n_z \geq 2$. From Eqs. (2-5) one can see that the scattering between different subbands makes $\pm\frac{3}{2}$ states mix with $\pm\frac{1}{2}$ states. Therefore, hole-phonon scattering due to the piezoelectric coupling makes contribution to the spin-flip scattering with or without strain.

In Fig. 4, we plot the SRT as function of $\epsilon_{\parallel}/\epsilon_{\parallel}^0$. It is seen from the figure that the SRT shows a minimum around $\epsilon_{\parallel}/\epsilon_{\parallel}^0 \sim -0.01$. This is because for large quantum well, the lift of the Γ -point degeneracy is very small and the lowest heavy-hole and light-hole states are very close to each other. Again, the SRT increases with the applied positive/negative strain due to the separation of the heavy hole and light hole states. Differing from the case of single subband, here the hole-phonon scattering due to the piezoelectric coupling makes strong contribution to the SRT even without strain. Nonetheless it is shown in the figure that when the strain $\epsilon_{\parallel}/\epsilon_{\parallel}^0$ is slightly deviated from -0.01 the SRT is mainly determined by the hole-phonon scattering due to deformation potential.

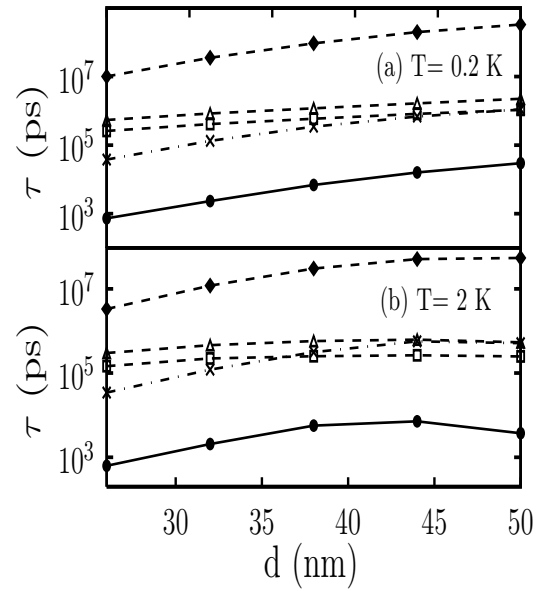


FIG. 5: SRT *vs.* the diameter d for QD's at $a = 20$ nm and $B = 1$ T under different strains. Curve with \bullet : $\epsilon_{\parallel}/\epsilon_{\parallel}^0 = 0$; \times : $\epsilon_{\parallel}/\epsilon_{\parallel}^0 = 0.07$; \square : $\epsilon_{\parallel}/\epsilon_{\parallel}^0 = -0.07$; \triangle : $\epsilon_{\parallel}/\epsilon_{\parallel}^0 = -0.09$; \blacklozenge : $\epsilon_{\parallel}/\epsilon_{\parallel}^0 = -0.3$. (a) $T = 0.2$ K; (b) $T = 2$ K.

In Fig. 5 we plot the SRT as a function of QD diameter d when $a = 20$ nm under different strains with solid curves for the strain-free case, chain curves for positive strain cases and dashed curves for negative strain cases. Similar to the case of small well width without strain in Fig. 1, for large well width without strain here the SRT also increases with the diameter for low temperature ($T = 0.2$ K) [Fig. 5(a)] and shows a maximum for higher temperature ($T = 2$ K) [Fig. 5(b)]. Strains keep these trends. Nevertheless for small negative strain $-0.2 < \epsilon_{\parallel}/\epsilon_{\parallel}^0 < 0$ the variations become smoother. This feature can be understood as follows: For negative strain the heavy hole states intercept with the light hole ones at high energies. The states around these intercepting points are particular efficient in spin relaxation. As said

in the previous section, the high energy states are arrayed very close to each other. The increase of diameter drives more states into the scattering channel and partly compensates the tendency of decrease. For larger negative strain ($\epsilon_{\parallel}/\epsilon_{\parallel}^0 < -0.2$), the heavy and light holes are separated again and the change of the SRT with the diameter becomes fast again as shown in the figure.

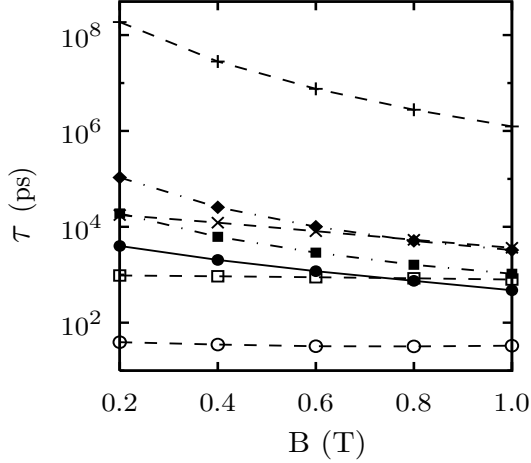


FIG. 6: SRT *vs.* the magnetic field B for a QD in (001) quantum well at $a = 20$ nm, $d = 20$ T and $T = 4$ K under different strains. Curve with \bullet : $\epsilon_{\parallel}/\epsilon_{\parallel}^0 = 0$; \blacksquare : $\epsilon_{\parallel}/\epsilon_{\parallel}^0 = 0.01$; \blacklozenge : $\epsilon_{\parallel}/\epsilon_{\parallel}^0 = 0.03$; \circ : $\epsilon_{\parallel}/\epsilon_{\parallel}^0 = -0.01$; \square : $\epsilon_{\parallel}/\epsilon_{\parallel}^0 = -0.02$; \times : $\epsilon_{\parallel}/\epsilon_{\parallel}^0 = -0.03$; $+$: $\epsilon_{\parallel}/\epsilon_{\parallel}^0 = -0.2$.

The SRT as a function of magnetic field B under different strains at $T = 4$ K is plotted in Fig. 6. As shown in Eqs. (30) and (31), the spin mixing is enhanced with the increase of the magnetic field. Therefore τ decreases with B . Moreover, similar to the case of the diameter dependence of the SRT, one finds that the τ - B dependence becomes weak when a negative strain is in the range $-0.2 < \epsilon_{\parallel}/\epsilon_{\parallel}^0 < 0$. This is because when the heavy-hole states intercept with the light-hole ones, Zeeman splitting which appears in the denominators of the spin mixing coefficients [*e.g.*, in the denominators of Eqs. (30) and (31)] becomes important which partially compensates the increase of the spin mixing with the magnetic field (*ie.*, B in numerators of spin mixing coefficients). Therefore, the SRT changes with B slowly. However, for a larger negative strain which makes a big separation between the heavy hole and light hole states, the τ - B dependence becomes stronger again.

B. QD's in (111) quantum well

We now turn to investigate QD's under different strains in (111) quantum well. As pointed out before, differing from the case of (001) quantum wells, there always exists spin mixing between spin-up and -down heavy (light) holes in the eigen functions of the Luttinger Hamiltonian

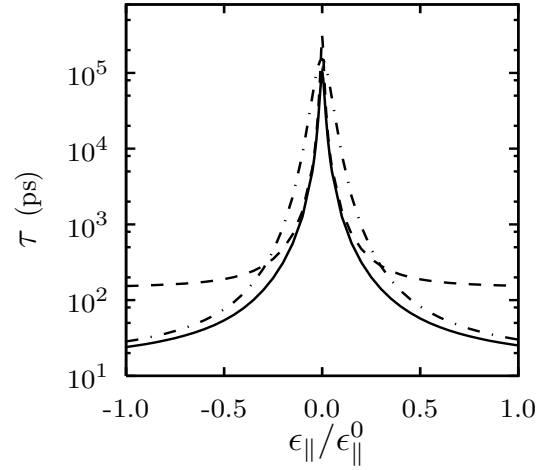


FIG. 7: SRT *vs.* strain at $a = 5$ nm, $d = 20$ nm, $B = 1$ T and $T = 4$ K. Solid curve: total SRT; Chain curve: SRT induced by the hole-phonon scattering due to piezoelectric coupling; Dashed curve: SRT induced by the hole-phonon scattering due to deformation potential.

of (111)-oriented quantum wells. Therefore, hole-phonon scattering due to both deformation potential and piezoelectric coupling contributes to the spin relaxation even there is no strain on QD. Moreover, the effect of strain on (111)-oriented crystal is also different from the (001) case: The strain hardly changes the relative position of energy levels of heavy and light holes, but introduces additional spin mixing which leads to additional spin relaxation.

In Fig. 7 we plot the SRT versus $\epsilon_{\parallel}/\epsilon_{\parallel}^0$ in a QD of $a = 5$ nm, $d = 20$ nm and $B = 1$ T at $T = 4$ K. It is seen from the figure that opposite to the (001) case as shown in Figs. 3 and 4, here the SRT *decreases* rapidly with the increase of strain in both positive and negative directions. This is because that the additional spin mixing introduced by the strain is the main effect in the present case, which makes the scattering rate increases with strain. Moreover, one finds that for small strain, the SRT is determined by the hole-phonon scattering due to deformation potential but after $|\epsilon_{\parallel}/\epsilon_{\parallel}^0| > 0.1$, hole-phonon scattering due to the piezoelectric coupling starts to contribute to the spin relaxation and after $|\epsilon_{\parallel}/\epsilon_{\parallel}^0| > 0.3$ it takes over the scattering due to the deformation coupling and becomes the leading contribution. However both contributions should be included in the calculation when strain is presented in (111) quantum wells.

We discuss the diameter and magnetic field dependence of SRT under different strains. In Fig. 8 the SRT is plotted against the QD diameter d for different strains. As the SRT with positive and negative strains are symmetrical, we only show the case with $\epsilon_{\parallel}/\epsilon_{\parallel}^0 \geq 0$. It is noted that when $\epsilon_{\parallel}/\epsilon_{\parallel}^0 = 0.12$ the hole-phonon scattering due to the deformation potential is dominant but when it is 0.28 the scattering due to the piezoelectric coupling becomes more important. Similar to the cases in the previous sections, the SRT increases with diame-

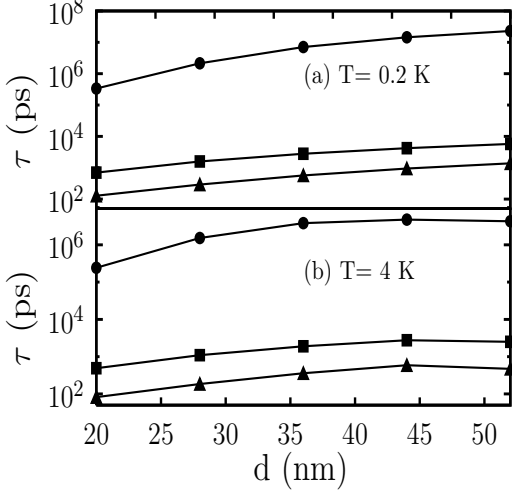


FIG. 8: SRT *vs.* the diameter d for a QD in (111) quantum well at $a = 5$ nm and $B = 1$ T under different strains. Curve with \bullet : $\epsilon_{\parallel}/\epsilon_{\parallel}^0 = 0$; \blacksquare : $\epsilon_{\parallel}/\epsilon_{\parallel}^0 = 0.12$; \blacktriangle : $\epsilon_{\parallel}/\epsilon_{\parallel}^0 = 0.28$. (a): $T = 0.2$ K, (b) $T = 4$ K.

ter monotonously when $T = 0.2$ K [Fig. 8(a)] and has a maximum when $T = 4$ K [Fig. 8(b)].

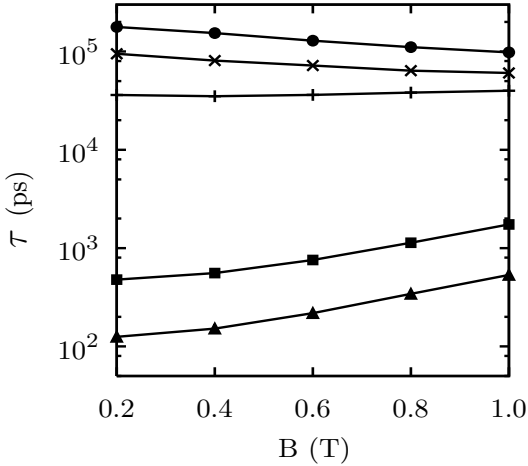


FIG. 9: SRT *vs.* the magnetic field B at $a = 5$ nm, $d = 20$ nm and $T = 4$ K under different strains. Curve with \bullet : $\epsilon_{\parallel}/\epsilon_{\parallel}^0 = 0$; \times : $\epsilon_{\parallel}/\epsilon_{\parallel}^0 = 0.01$; $+$: $\epsilon_{\parallel}/\epsilon_{\parallel}^0 = 0.02$; \blacksquare : $\epsilon_{\parallel}/\epsilon_{\parallel}^0 = 0.12$; \blacktriangle : $\epsilon_{\parallel}/\epsilon_{\parallel}^0 = 0.28$.

In Fig. 9 we show the magnetic field dependence of the SRT under different strains. When there is no strain or very small strain, similar to the case of QD in (001) quantum well and our previous investigation on electron spin in QD's,¹⁰ the SRT decreases with the magnetic field. However for a little bigger strain the SRT *increases* with the magnetic field. This is understood that the spin mixing induced by strain in (111) quantum well makes a major contribution to the spin relaxation for sufficient big strain. Nevertheless, this mixing *decreases* with B .

This can be seen in following: In the case when there is no inter subband spin mixing and the heavy- and light-hole states are separated from each other, then almost all the spin mixing comes from the off-diagonal terms of the strain Hamiltonian [Eqs. (10) and (11)]. Using the perturbation method, and adopting the lowest four states of H_0 as basis, the wave functions are written into:

$$\begin{aligned} \langle \mathbf{r} | \Psi_{\uparrow} \rangle &= \langle \mathbf{r} | 0, 0, 1, \frac{3}{2} \rangle + \mathcal{C} \langle \mathbf{r} | 0, 0, 1, \frac{1}{2} \rangle + \mathcal{D} \langle \mathbf{r} | 0, 0, 1, -\frac{1}{2} \rangle, \\ \langle \mathbf{r} | \Psi_{\downarrow} \rangle &= \langle \mathbf{r} | 0, 0, 1, -\frac{3}{2} \rangle + \mathcal{E} \langle \mathbf{r} | 0, 0, 1, \frac{1}{2} \rangle \\ &\quad + \mathcal{F} \langle \mathbf{r} | 0, 0, 1, -\frac{1}{2} \rangle, \end{aligned} \quad (34)$$

in which $\mathcal{C} = m_0 H / (\hbar e B \kappa + \Delta \epsilon)$, $\mathcal{D} = m_0 I / (2 \hbar e B \kappa + \Delta \epsilon)$, $\mathcal{E} = -m_0 I^* / (2 \hbar e B \kappa + \Delta \epsilon)$ and $\mathcal{F} = m_0 H^* / (\hbar e B \kappa + \Delta \epsilon)$ with $\Delta \epsilon = 2 \gamma_2 \hbar \Omega - 4 \gamma_2 \frac{\hbar^2 \pi^2}{m_0 a^2}$. H and I are the matrix elements of strain Hamiltonian [Eqs. (10) and (11)], which are independent of the magnetic field. Consequently the spin mixing decreases with B .

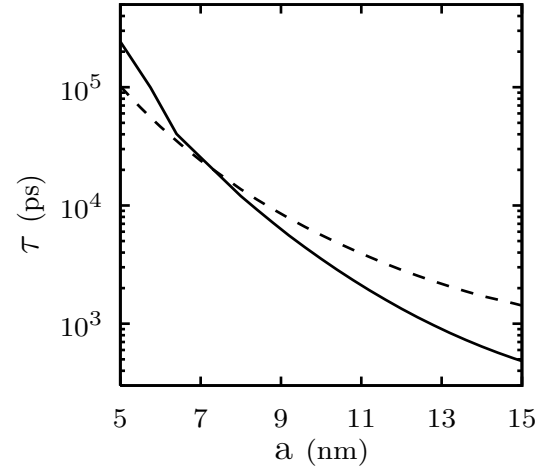


FIG. 10: SRT versus the well width a at $d = 20$ nm, $B = 1$ T and $T = 4$ K. Solid curve: (001) quantum well; Dashed curve: (111) quantum well.

C. Well width dependence of the SRT

Finally we investigate the quantum well width dependence of the SRT of QD's with $d = 20$ nm and $B = 1$ T at $T = 4$ K. The SRT's of QD's in (001) and (111) quantum wells are plotted as function of quantum well width a . It is seen that for both cases the SRT's decrease with the well width, which is totally opposite to the cases of electron spin in QD's¹⁰ and quantum wells.¹⁸ This difference originates from the fact that for electron spin the spin-orbit coupling decreases dramatically with the well width.^{10,18} Nevertheless, for hole spin although the spin-orbit coupling also decreases with a [see Eqs. (5) and (16)], the decrease of the intervals between different energy states is faster [see Eqs. (4) and (15)]. Consequently

more states are included in the spin-flip scattering channel and τ decreases with the well width.

IV. CONCLUSIONS

In conclusion, we have performed a comprehensive investigation on hole spin relaxation in GaAs QD's confined in quantum wells along (001) and (111) directions by exactly diagonalizing the hole Luttinger Hamiltonian.

We find for QD's in (001) quantum wells with small well width where only the lowest subband is involved, the SRT *increases* with the QD diameter at very low temperature (*e.g.*, 0.2 K) or first increases until it reaches a maximum and then decreases at higher temperature (*e.g.*, 4 K). These features are opposite to those of electron spin in QD's. Moreover, unlike the case of electron spin where the SRT is mainly determined by the electron-phonon scattering due to the piezoelectric coupling, here only the hole-phonon scattering due to the deformation potential contributes to the spin relaxation. Strain changes the relative positions of energy levels of heavy hole and light hole. A positive strain increases the energy gap between heavy hole and light hole and enhances the SRT. A negative strain decreases the gap and reduces the SRT until the interchange of the lowest energy states from heavy hole to light hole. After that the SRT increases again. Moreover, very close to the interchange point, as the energy levels of heavy hole and light hole are very close to each other, the hole-phonon scattering due to piezoelectric coupling contributes to the spin relaxation too. For large well width where multi-subband effect is important, hole-phonon scattering due to the piezoelec-

tric coupling contributes to the spin-flip scattering with or without strain. Nevertheless the SRT is still mainly determined by the scattering due to deformation potential except at the interchange point. The magnetic field dependence of the SRT is also discussed.

For QD's in (111) quantum well things are quite different from those for QD's in (001) quantum well: Hole-phonon scattering due to both piezoelectric coupling and deformation potential contributes to the spin relaxation and should be both included in the calculation, regardless of the well width; Strains can hardly change the relative positions of energy levels of heavy hole and light hole but introduce *additional* spin mixing. Therefore the SRT decreases rapidly with strain; The SRT decreases with magnetic field like the case of QD in (001) quantum well and our previous investigation on electron spin in QD's when there is no strain or very small strain. However for strain which is big enough that the spin mixing is mainly determined by it, the SRT *increases* with B .

Finally we show that the hole SRT decreases with well width for QD's in both (001) and (111) quantum wells which is totally opposite to the cases of electron spin in QD's and quantum wells.

Acknowledgments

This work was supported by the Natural Science Foundation of China under Grant No. 90303012. MWW was also supported by the "100 Person Project" of Chinese Academy of Sciences and the Natural Science Foundation of China under Grant No. 10247002. He would like to thank B. F. Zhu for valuable discussions.

* Author to whom correspondence should be addressed; Electronic address: mwwu@ustc.edu.cn.

† Mailing Address.

¹ *Semiconductor spintronics and quantum computation*, ed. by D. D. Awschalom, D. Loss, and N. Samarth (Springer-Verlag, Berlin, 2002).

² I. Žutić, J. Fabian, and S. Das Sarma, *Rev. Mod. Phys.* **76**, 323 (2004).

³ M. Valín-Rodríguez, A. Puente, and L. Serra, *Phys. Rev. B* **66**, 235322 (2002).

⁴ J. A. Gupta and D. D. Awschalom, *Phys. Rev. B* **59**, R10421 (1999).

⁵ A. V. Khaetskii and Yu. V. Nazarov, *Physica E* **6**, 470 (2000).

⁶ B. Hackens, F. Delfosse, S. Faniel, C. Gustin, H. Boutry, X. Wallart, S. Bollaert, A. Cappy, and V. Bayot, *Phys. Rev. B* **66**, 241305 (2002).

⁷ A. V. Khaetskii and Y. V. Nazarov, *Phys. Rev. B* **61**, 12639 (2000).

⁸ A. V. Khaetskii and Y. V. Nazarov, *Phys. Rev. B* **64**, 125316 (2001).

⁹ L. M. Woods, T. L. Reinecke, and Y. Lyanda-Geller, *Phys. Rev. B* **66**, 161318(R) (2002).

¹⁰ J. L. Cheng, M. W. Wu, and C. Lü, *Phys. Rev. B* **69**, 115318 (2004).

¹¹ L. M. Woods, T. L. Reinecke, and R. Kotlyar, *Phys. Rev. B* **69**, 125330 (2004).

¹² J. M. Luttinger, *Phys. Rev.* **102**, 1030 (1956).

¹³ H. R. Trebin, U. Rössler, R. Ranvaud, *Phys. Rev. B* **20**, 686 (1979).

¹⁴ G. L. Bir and G. E. Pikus, *Symmetry and Strain-Induced Effects in Semiconductors* (Wiley, New York, 1974).

¹⁵ S. H. Park and S. L. Chuang, *J. Appl. Phys.* **87**, 353 (2000).

¹⁶ I. K. Oh and J. Singh, *J. Phys.: Condens. Matter* **13**, 10851 (2001).

¹⁷ *Numerical Data and Functional Relationships in Science and Technology, Landolt-Börnstein, New Series*, edited by O. Madelung, M. Schultz, and H. Weiss (Springer-Verlag, Berlin, 1982), Vol. 17.

¹⁸ M. Q. Weng and M. W. Wu, *Phys. Rev. B* **68**, 075312 (2003).